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AIR RESOURCES BRANCH

AIR QUALITY MONITORING SECTION

Scientific Review Panel Comments on ERT/MEP Mathematical Modelling Plan

ARB-46-82-AQM

Compiled for the

Ontario Ministry of the Environment
880 Bay Street
Toronto, Ontario

By

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Environment Canada / Environnement Canada

Atmospheric Environment Service / Service de l'environnement atmosphérique

4905 Dufferin Street
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SEP 16 1982 RECD

September 3, 1982

Dr. S. Stevens
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Dear Dr. Stevens:

Enclosed are comments and recommendations on the final ERT/MEP proposal to the Ontario Ministry of Environment. After the September 23 and 24 SCIREP meeting, I may have more specific comments to add.

Yours sincerely,

Leonard A. Barrie

Encl.

COMMENTS AND RECOMMENDATIONS ON THE ERT/MEP MESOSCALE - LRTAP MODEL PROPOSAL OF AUGUST 1982

BY

L.A. BARRIE

GENERAL COMMENTS

As this reviewer understands it the model will consist of two sub-models: a Long Range Transport one covering 4000 km at 1^{o} lat.-long. resolution and a Mesoscale one good out to 500 km of a source with 0.1^{o} lat.-long. resolution. The models will be on a 32 x 32 grid with 12 vertical layers up to 5 km. The operating time in an unvectorized mode is 0.25 to 1 of real time and in a vectorized mode 0.025 to 0.1 of real time. The slowness of computation is due to the large number of processes being modelled in more detail than has been done prior to now by other models. However, it represents a real drawback as far as development is concerned. In order to be able to predict acidic deposition on the long term (objectives 1 and 2), the model would have to produce output for periods of time ranging from a month to a year (shorter time periods are inadequate since existing precipitation chemistry networks cannot accurately resolve acidic deposition fields for averaging periods less than a month). Performing at a relatively fast rate of 0.1 of real time, it would take a month or more to produce a single prediction for a single year. This leaves little for development. Thus the full-blown model will likely be used

for predictions of episodes of 3-5 days than for long term analyses. It is a property of precipitation chemistry measurements and parameterizations of wet scavenging characteristics that they become more accurate the longer the averaging period of measurements or model predictions. For a short period of 3-5 days they are highly uncertain. Consequently, the model used on a 3-5 day period will be restricted to dry periods. In other words, it becomes a 'dry oxidants model'. It will remain an oxidants model unless simplification of transformation and removal processes are made to expedite faster computation, thereby enabling one to generate long term deposition fields. It should be emphasized however that such a Long Range Transport acid deposition model would simulate transport more accurately than existing lagrangian models but will not provide a more accurate representation of non-linear chemical processes because of over simplifications to save computational time. Thus it would be open to the same criticism about non-linearity as present models are.

The above comments are not so much a criticism of the proposal as they are a description of limitations that all modellers must work under and all contracting agencies should be aware of.

In the proposal it was unclear whether the Long Range Transport model would be run after having solved 'the home grid-square' problem with the mesoscale model. In order to improve on past modelling efforts this should be done.

SPECIFIC COMMENTS

Wet Deposition

1. equation 7-14 is incorrect.

2. page 7-20, the solubility of most gases is higher at lower temperatures not lower as indicated.

3. Note that the scavenging ratio approach is an empirical, stochastic one which necessarily requires averaging over many events to be accurate. As mentioned in the general comments this places a lower limit on the averaging time of a model's prediction of wet deposition.

4. Parameterizations of dry deposition are, on the whole, good ones. The best values of r_s and r_d to use, should be established by conducting a more extensive literature survey.

Sensitivity Tests

5. It is disturbing that 'differences seen between the two simulations' (numerical integration schemes) 'are, in fact, greater than those seen in the model formulation sensitivity analysis'. Comments from numerical analysis experts should be solicited and heeded.

CONCEPTS OF MODEL EVALUATION (CHAPTER 11)

6. The contents of this section are very theoretical. Little effort has been made to outline in detail objective tests that will be performed to demonstrate to the contracting agency that the model is performing within a specified degree of precision.

7. With regard to the last sentence: 'the acceptability of the two models will be determined by the expertise and experience of the scientific team working on the project'. All the expertise in the world is useless if the final product does not pass the ultimate test of reproducing within a certain degree of certainty the observations. The contracting agency must insist on such tests being performed.

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OCT - 1 1982 RECD

September 28, 1982

Dr. S. Stevens
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Dear Dr. Stevens:

Enclosed are some comments on the recent ERT/MEP modelling proposal which was reviewed by the scientific review panel on September 23 and 24, 1982. These comments are in addition to those sent to you by mail on September 3 which can be considered unchanged. I hope they prove useful in deciding the nature of the next phase of the modelling effort.

Yours sincerely,

L. A. Barrie

Leonard A. Barrie

Encl.

COMMENTS ON THE ERT/MEP EULERIAN MODEL PROPOSAL OF AUGUST 1982

by L.A. Barrie

The modelling effort proposed will be an initial step in the long journey towards the goals outlined in the Ontario Ministry of Environment's objectives. In order for that step to be a firm one, action should be taken on several fronts:

1. it is essential that the modelling group's meteorological support be bolstered, possibly by sub-contracting to a reputable university group for mesoscale modelling and enlisting the services of the Atmospheric Environment Service for synoptic scale meteorology.
2. the sponsoring agencies need to specify in detail the main applications to which it requires the model to be put. In particular, it should be explicitly stated that for control purposes wet and dry deposition rates of sulphates and nitrates are required in eastern North America on a seasonal basis for at least a year.
3. the sponsors should ensure that the data base against which model predictions are tested and checked be certified by the producers of that data. If possible the data base should be a standard one against which many models are run.

4. the sponsors should proceed with the model under the condition that the SCIREP committee's recommendation be acted upon. A probabation period of a year would give ERT/MEP sufficient time to act on the recommendations and to develop and test sections of the model.

5. the sponsors should determine what emissions inventories are required and then take steps to encourage their compilation within the next two years.

6. A large computer on which to operate the model needs to be arranged. This is essential if a model analysis on an annual basis is to be performed.

The sponsor should realize that in two years time the most that one can expect from any modelling group is a preliminary model that has been tested using monthly data bases from small portions of the large scale modelling domain and possibly annual wet deposition data bases for the whole domain. Present monitoring efforts in North America do not provide a complete set of air and precipitation chemistry measurements but rather only one for precipitation. Thus the model will not be suitable for use in court but it will be approaching a level of 'reality' that is higher than existing lagrangian models.

It is extremely important to our understanding of the atmospheric cycle of acids and oxidants that this modelling effort be undertaken.

OCT - 4 1982 RECD

SUMMARY OF EVALUATION OF ERT PROPOSAL "MODELS FOR LONG RANGE AND MESOSCALE TRANSPORT AND DEPOSITION OF ATMOSPHERIC POLLUTANTS" August, 1982

From Jack G. Calvert, NCAR, Boulder, CO 80307

The ERT Modeling System Design documents developed in response to the request of the Ontario Ministry of the Environment appear to be well prepared. This effort is significantly better than that shown in preliminary efforts which were reviewed by this panel some months ago. The present comments should supplement the detailed comments on the atmospheric chemistry sections which were made by me in my September 7th, 1982 letter to Dr. Sam Stevens of Concord Scientific Corp; copy attached.

The plan is judged according to the following four levels of success which were outlined at the SCIREP Meeting:

1) Sufficiently accurate for strategy formulation; legally defensible
2) Diagnostically and qualitatively useful tool.
3) Stimulates advances toward level 1.
4) Forget the project for now.

The chemistry sections are well-conceived, up-to-date on the literature cited, and they offer a reasonably high degree of sophistication in the handling of the chemical input to the program, with the exception of the problem areas outlined in the Sept. 7, 1982 letter from me (specifically points 1, 11, 17, 18, 19, 20, and 21 are seemingly significant).

The programs for transport and cloud interations in the ERT report seem less complete and useful for quantitative efforts (surmised from the committee discussions).

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September 7, 1982

Dr. Sam Stevens
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Dear Sam:

I have had a chance to read the ERT Modeling System Design Documents which they developed in response to the Canadian Government contract. On the whole the document is quite impressive, and it is a very great improvement over the preliminary efforts of ERT reviewed some months ago. There are a few comments (some trivial) which the contractors may wish to consider before the review meeting this month:

1) The results of the 1-day scenarios using the present model show little, if any, deviation from linearity in $SO_2 \rightarrow SO_4^=$. Is this expected? Is it the result from high SO_2 emissions over the grid employed and dominance of local sources? Have any scenarios for 3-4 day transport over regions low in emissions been tested similarly?

2) Table 6.2-2: $k_a \backslash (k_a + k_b) = 0.37 \pm 0.88$ (?) for n-hexane.

3) Table 6.2-3: Caption (at room temperature and pressure?)

4) Page 6-16: bond on wrong carbon, line 5.

5) Page 6-17: equation (6.2.28a) bond in species after →.

6) Page 6-19: below mid-page: bond to wrong carbon in peroxy radical.

7) Page 6-21: top line: (∿20-40%) from where? Most recent work gives ∿37% from two laboratories (1 atm).

8) Page 6-22: top line; Akimoto et al. should be referenced here as well (J. Phys. Chem., 85, 2249 (1981)).

9) Page 6-28: The rationale behind neglecting C_6H_6 chemistry is unclear. Certainly the CH_2O formation from $(HCO)_2$ would be important

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in stimulating O_3 generation, etc. The absence of free radicals from $(HCO)_2$ photochemistry may be made up for through the CH_2O product reactions.

10) Table 6.2-5: What are the magnitudes of β's used for given solar zenith angle?

11) Do the developers of the reaction scheme 1-84 see any problems with the reaction 81 as written (p 6-42)? All of the evidence that I know of points to a chain propagation following $HO+SO_2$, and the chain termination implied by 81 can lead to very different effects. The arguments given on p. 6-52 are not compelling. Somehow radical-radical interaction (two $HOSO_2$'s, $HOSO_2O_2$'s, . . .) is expected here? Saying that $HSO_3 \rightarrow SO_4$ is very fast in the presence of air does not eliminate the problem.

12) Page 6-54: Is it not more reasonable to assume O_3 + NO is more like CH_2O_2 + NO than CH_3O_2 + NO since the theoretical thermal properties of O_3 and CH_2O_2 are very similar (Goddard)?

13) Page 6-56, line 7; proper reference to Whitbeck's study (not review) could be his thesis or better: NBS Spec. Publ. (U.S.), 526, 212-214 (1978); here he gives the experimental results of the tert-BuO_2 + SO_2 system.

14) Page 6-56, line 12: Remove word, "Both".

15) Page 6-61, line 7: Word correct? "remaining".

16) Table 6.3-2; reference to data?

17) Figure 6.4-1; p. 6-99: Is the $HONO_2/SO_4^=$ ratio calculated here in accord with measured ratios?

18) Page 6-107; end middle paragraph: Is the NO_x full oxidation reasonable in a real world where NO_x emissions continue over most of the area? It appears to me that the H_2O_2 generation is very dependent on these choices.

19) What is the main justification for using the chemical scheme as presented rather than the "Carbon Bond-III" mechanism which appears to have similar positive features in dealing with the hydrocarbon reactivity?

20) Page 6-113: Present evidence seems to favor the possible significance of $N_2O_5 + H_2O\ (\ell) \rightarrow 2HONO_2$ reaction in the cloud water. Is it correct to ignore this as stated on the top of p. 6-113?

21) P. 6-114: It is not clear from the comments or the approach of cloud treatment to be used by the contractor how they will judge the amount of air which can be processed in a cloud in a given time period.

22) Table 6.6-2: HSO = HSO_3^-? Is NO_3^- present here also as an aqueous phase species?

I trust these comments will be of some use to the contractors, and I look forward to seeing you and them soon.

Best wishes,

Jack Calvert
Senior Scientist
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JGC/smh

DET NORSKE METEOROLOGISKE INSTITUTT

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SEP 17 1982 RECD

Deres ref.	Vår ref. (bes oppgitt ved svar)	Dato
	342/3807/82 AE/MB	8 September 1982

Dear Dr. Portelli,

Enclosed please find my comments to the Phase 1 Modelling System Design Reports.

Best regards

Anton Eliassen

Anton Eliassen
Senior scientist

Encl.

Brev adresseres til Det norske meteorologiske institutt, ikke til funksjonærer.

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COMMENTS TO THE ERT/MEP MODELLING SYSTEM DESIGN REPORT OF AUGUST 1982

1. General impression

The planning of the model design seems to be well done. Indeed, in most respects we seem to approach a model that includes, as far as possible, the present knowledge in meteorology and air chemistry. The parts concerning the atmospheric boundary layer and the air/cloudwater chemistry gives a very good impression. The parts of the model design that relate to "synoptic meteorology" seem weaker. This deficiency is my main concern. In the following I will attempt to substantiate this point.

2. Wind field model

a) "Mass consistency"

On page 3-5 it is stated that "Since the dispersion model is of the Eulerian rather than Lagrangian type, the wind field must be mass consistent". This statement represents a misunderstanding. The requirement of a "mass-consistent" wind field is not a function of whether one chooses Eulerian of Lagrangian integration. The text goes on to point out that the winds used in the advection terms may or may not be a solution of the continuity equation. This must also be a misunderstanding, since no wind field on its own can violate the continuity equation. Wind fields can, however, imply unrealistic variations of the air density ρ, which imply unrealistic variations in pollutant concentrations, and therefore must be avoided. This is probably what is meant by making the wind field "mass consistent".

b) Barotropic-baroclinic

On page 3-18 it is stated that under barotropic conditions the heights of the pressure surfaces are constant and that air motion is horizontal. This is wrong. Barotropic conditions are defined as an idealized situation when pressure surfaces and density surfaces coincide (but are not necessarily horizontal). For an ideal gas, this also means that surfaces of constant temperature, or constant potential temperature, coincide with the pressure surfaces.

c) Radiosondes and CMC analysis

The basis for the upper air wind field will be the CMC wind analysis and the radiosonde data at 00 and 12 Z. It is not quite clear how one plans to merge these two sources of data. From Figures 3.4 and 3.5 one may infer that the 00 and 12 Z wind fields are obtained directly from the radiosondes, whereas the 06 and 18 Z wind fields are obtained from the CMC analysis. Such a procedure is unfortunate since the 00 and 12 GMT wind fields might have other properties than the 06 and 18 Z wind fields. CMC has, of course, used the radiosonde data in their 00 and 12 Z analyses, probably in the usual manner together with a 12-hour prog as a first guess for the analyses. It is difficult to see how a wind analysis based only on radiosonde information can be better than the CMC analysis, which automatically carries information from previous observations.

d) Calculation of vertical velocity

Following up the discussion under c), it is my guess that the vertical velocities estimated at 06 and 18 Z from the CMC analyses will be better than those based only on radiosonde data, i.e. the 00 and 12 Z values. When operating a weather prediction model based on the so-called primitive equations, the analysed fields are adjusted so that the wave motions that have phase speeds much larger than the usual

meteorological systems are kept small in amplitude. This process, which is called initialization, is usually carried out by more sophisticated methods than assuming that the error in $\left(\frac{\partial u}{\partial x}\right)_p + \left(\frac{\partial v}{\partial y}\right)_p$ is proportional to $|\vec{v}|$.

3. LRT and Mesascale model

a) Wet deposition

The modelling system design report contains a good chapter on atmospheric chemistry associated with acid precipitation (chapter 6). In spite of all that is known about the chemistry in clouds, it is stated, and I think correctly, that "It will be some time before a washout parameterization can fully account for the complex chemistry in clouds". The regrettable situation is that at the moment one has to accept a wet deposition formulation for reactive gases based on scavenging ratios which are not linked with the chemical state of the cloud. If, in the course of this modelling exercise, one could find a better solution, it would be a great step forward.

Even if the problem of calculating correct scavenging ratios was solved, the problems relating to the temporal and spatial "patchiness" of precipitation events remain. The importance of good time and space resolution becomes clear if we consider a long-term average ($\sim$ annual) wet deposition pattern. A key parameter in the determination of such a pattern is the average residence time T_p for the pollutant with respect to wet deposition. Given the transport winds, then T_p , together with the corresponding residence time T_d for dry deposition, determine how far the pollutant travels, and hence the deposition patterns.

Following Rodhe and Grandell (1972, 1981) we assume a constant scavenging coefficient λ_p to apply during precipitation. For sulphur, λ_p^{-1} is of the order 1 hour. If we think of the sequence of dry and wet periods experienced by a pollutant-carrying particle or trajectory, the rate of wet

removal that applies may be taken as a stochastic process $\lambda(t)$ defined by

$$\lambda(t) = \begin{cases} 0 \text{ if dry period at } t \\ \lambda_p \text{ if precipitation occurs at } t \end{cases} \quad (1)$$

Assuming now that $\lambda(t)$ is a Markov process with stationary transition probabilities, the lengths of the dry and wet periods are exponentially distributed. If τ_d and τ_p are the average lengths of dry and wet periods experienced by the moving particle, it can be shown that the average residence time T_p for the pollutant with respect to wet deposition is

$$T_p = \tau_d p_d + \frac{\tau_d + \tau_p}{\tau_p} \cdot \frac{1}{\lambda_p} \quad (2)$$

where p_d is the probability of a dry period at the starting point of the moving particle. Given the transport winds then T_p, together with the corresponding residence time T_d for dry deposition, determine the deposition of pollutant as a function of travel distance.

Relationship similar to (2) may be derived with slightly other assumptions, see Rodhe and Grandell (1981). The quantities τ_d and τ_p have been estimated by Hamrud et al. (1981) from trajectories and precipitation data. τ_d was found to be 51 hours in summer and 53 hours in winter, whereas τ_p was 11 hours in both cases. If we take τ_d = 50 hours, τ_p = 10 hours, λ_p^{-1} = 1 hour and approximate the Eulerian probability from the Lagrangian data, i.e.

$$p_d \approx 1 - \frac{\tau_p}{\tau_d + \tau_p} = 0.83$$

then (2) yields

$$T_p = 50 \text{ hours} \cdot 0.83 + 6.1 \text{ hour} = 47.5 \text{ hours}$$

This shows that for pollutants that are relatively efficiently removed during rain, such as sulphur, the average length of a dry period is a key quantity for the determination of T_p, and

hence for the wet deposition pattern. T_p is less sensitive to λ_p: if λ_p is changed by a factor of two in either direction, T_p varies between 44.5 and 53.5 hours. It is noteworthy that the complicated chemistry enters into λ_p only, whereas the more important quantity τ_d is related to synoptic meteorological data.

It is therefore important that the precipitation data used by any model imply a correct value of T_p. This may be difficult to achieve, due to the time and space resolution of precipitation data available from the WMO station network. In Europe, precipitation amounts are generally measured in periods of 12 or 6 hours. The spacing of the stations available on the WMO telecommunication network is such that a 150 km grid element over land will contain two to three reporting stations on the average. If the calculations are based on gridded precipitation amounts, these are averaged out in time and space, with overestimated duration and underestimated intensity. For a trajectory moving through such a precipitation field, τ_d will be too short, perhaps leading to an incorrect value for T_p.

I am rather surprised to see that hourly precipitation data are available (p. 1-75). Such data are practically non-existent in Europe. If the spatial resolution of these data is also reasonably dense, this will help to generate realistic values of τ_d. A map showing stations with such data would be helpful.

b) Model sensitivity tests

The tests with the long range transport model clearly show the importance of the numerical advection scheme. The differences in model results with different schemes are so large that sophisticated features in the model may be masked by advection errors. However, the work on this problem seems well under way (chapter 5).

Compared to the tests with the numerical advection scheme, the other sensitivity tests produce relatively small changes in the calculated values. If one had the task of picking out the model version that was best in reproducing some set of measured sulphur data, the result could easily have been inconclusive. In other words, the sensitivity to variations in key parameters is disappointingly small.

c) What species are important to model in "acid rain" modelling?

It is interesting to note that linear chemistry seems to work rather well as far as SO_x is concerned, but leads to unacceptabel errors for NO_x and PAN, for example. Scandinavia ecologists claim that the deposition of sulphur is the important acidifying mechanism, since sulphur, in the long run, passes through the ecological soil system and comes out in the stream as sulphate. This sulphate will of course carry cations with it, because of the electroneutrality condition. The cations will often be H^+-ions, as a result of ion exchange between the precipitated water and the soil. Nitrate is not as important, since it to a large extent is taken up by plants, little coming out in the streams and rivers. This view is to a certain extent opposed by British scientists. My point here is the following: Facing the very complicated atmospheric chemistry, the scientists dealing with effects of acid rain should indicate what components should be modelled. If sulphate is the main acidifying agent, then our task becomes considerably simpler since linear chemistry seems to be sufficient.

(Clearly, this remark applies only to "acid rain" modelling, not to oxidant modelling.)

4. Conclusions

My main critisism relates to how the synoptic meteorology has been taken care of. I doubt that the wind field generation scheme is good enough. More weight should be

put on finding out when and where it rains. This seems to be at least as important as finding the correct scavenging ratio for a certain precipitation event. How will the presence of clouds be included?

In general, however, the design plan for the model represents a major effort to combine the existing knowledge in a variety of different fields of atmospheric science. Complexity does not automatically lead to measurable improvement, but the more specific modelling of the different atmospheric processes is our best chance. As a whole, the modelling system design reports submitted by MEP and ERT represent an admirable step in the right direction. I therefore recommend that the project should continue.

References

Hamrud, M., H. Rodhe and J. Grandell, 1981. A numerical comparison beteen Lagrangian and Eulerian rainfall statistics. Tellus 33, 235-241.

Rodhe, H. and J. Grandell, 1972. On the removal time of aerosol particles from the atmosphere by precipitation scavenging. Tellus 24, 442-454.

Rodhe, H. and J. Grandell, 1981. Estimates of characteristic times for precipitation scavenging. J. of the Atmos. Sci. 38, 370-386.

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Comments arising from the second meeting of SCIREP,
23 - 24 September 1982 in Toronto.

I. Precipitation and Clouds

In the modelling system design report, little was mentioned about the cloud and precipitation data to be used as model input. During the meeting it was stated that extensive data from a radar network was available. My original doubts on this point are therefore partly resolved. The radar data should cover the complete grid.

II. Wind Field on the Synoptic Scale

In my comments to the design report I have up problems associated with the method proposed to construct the wind field. I still think this is a very serious problem. However, if AES joins the programme one could base the wind field more on CMC products where the winds have been "initialized" so that the non-meteorological modes are not present. Another possibility is to use the ω-equation. In any case it is absolutely necessary to improve on this point. I refer to my comments on the project plan for further details.

III. Initial Concentrations

In episode studies, the integration of the model must always start long enough before the episode to be studied, so that the calculated concentrations during the episode are completely independent on the assumed initial concentrations. Only then will one get a correct evaluation of model performance when calculated and measured data are compared.

IV. Measured Data

At the first SCIREP meeting I took up the difficulties associated with using measured data from different programmes for comparison with calculated data. D ta arising from different programmes will generally have different properties (error characteristics). Our experience in Europe shows that in many cases this will limit the obtainable agreement between measured and calculated data. It seems that little further thought has been given to this point by the principal investigators.

V. Long Term Concentrations Versus Episode Studies

At the meeting it became clear that one plans to construct long-term (~ annual) deposition patterns from a limited number (~ 12-15) of episode studies covering 3-4 days. In practice this will be difficult to do. To cover the wet deposition pattern, one will have to include the important wet episodes in the model runs. In the wet episodes, however, the winds are atypical compared to the annual average, so the dry deposition in these cases will also be atypical. This effect is difficult to correct for, and therefore long-term calculated data obtained in this way will be easy to critisize. Regulatory application of the model will therefore be difficult. This way to construct long-term deposition patterns is not recommended.

If one has to study a large number of episodes anyway, in order to obtain "episode statistics", one might as well run the model for at least one year.

VI. Mesoscale Model

The present project plan is tilted towards specification of the long range transport model. Undoubtedly the model will be able to simulate long range transport. To extend the model to cover the mesoscale is difficult since this scale is not resolved by the routine meteorological observation network. It is my feeling that a good incorporation of mesoscale processes can only be achieved using a mesoscale dynamic model. This is a task that is very large with respect to both computer and personnel resources. At present the principal investigators do not have the necessary personnel resources to carry out this task, according to my best judgement.

The importance of describing the processes on the mesoscale depends on what time resolution is needed. For long term calculations, or for episode statistics, a resolution on the mesoscale is unnecessary.

VII. Conclusions

It is therefore my opinion that the programme be continued. For reasons stated under VI, however, it is felt that the mesoscale part of the programme should not be pursued unless very substantial economic resources are available and the team of principal investigators is augmented with an expert on dynamic mesoscale models. If the issues raised under I, II and cannot all be adequately handled, the project should be discontinued.

Comments on the ERT/MEP Report entitled "Model for Long Range and Mesoscale Transport and Deposition of Atmospheric Pollutants" (Dated: August 1982)

Submitted by:
Andrey Feuerverger Ph.D. (Statistics)
Toronto

Submitted to:
Concord Scientific Corporation
Re: SCIREP

September 1982

Statement of Purpose

This brief report summarizes our impressions of the following items which we have reviewed:

(a) written transcript of the March 23/24 discussions at O'Hare Ramada Inn. (251 pages)

(b) SCIREP pre & post meeting review comments Re: March 23/24. (13 reports)

(c) Statement of the objectives of the Mesoscale - LRTAP model development at OME. (1 page)

(d) ERT/MEP Phase 1 Modelling System Design report entitled "Models for Long Range and Mesoscale Transport and Deposition of Atmospheric Pollutants. (Vol. I, Vol. II, Executive Summary Volume)

We consider both our mandate and expertise to be limited to matters of statistical methodology. However, we have chosen to comment freely on other topics as well with the understanding that appropriate caveats are implicit in those cases.

We record here that the items (a) - (d) catalogued above are the only ones that have been available to us in our work on the present report.

Comments on the O'Hare Transcript

As we did not participate in the March 23/24 meeting, we found it necessary to read the written transcript in detail. We record here only a few brief impressions concerning some of the matters raised.

(a) page 5. OME indicates that "at the current time, the modelling should be used as one intricate tool among many tools to try to gain at least a relative assessment of the environment". This represents, in our view, a realistic assessment of the likely limitations of the modelling approach here.

(b) page 6. OME indicates specifically that it wishes to have some "development of the uncertainties" that arise in modelling approach.

(c) page 8. ERT indicates that they already have two long-range transport models: EPRI and SURADS, and speak of "putting together the next generation of models". Our first question here is whether these models are already adequate to OME's purpose. If not, it is fair to ask whether or not there is any basis for believing that the next generation will in fact be adequate. OME should also require a clear understanding of what they would be getting that actually will be new.

(d) page 15. ERT states that "one of the more important parts of this project is model validation" but does not indicate that ERT will use the services of a statistical expert to help them with this highly technical task.

(e) page 21. There is some discussion here of "interactive capability" for the "decision maker". This sounds like fancy trimming and a waste of money. It also contributes to the myth that an unknowledgeable decision-maker will somehow be able to make intelligent use of a complex and technical model. I cannot see anything about the proposed model that suggests that it could be

run and interpreted by anyone less than an expert. Similar comments re: pages 36-37.

(f) page 56. Dr. Lamb suggests accepting the fact that "atmospheric motion has a stochastic nature".

(g) page 91. Dr. Lumley stresses the need for a clear statistical analysis in view of the fact that the model is intended for regulatory purposes, and that one cannot know if the physics in the model is actually right.

(h) pages 102-104. There is a distressing amount of confusion here concerning the testing and adjustment of models on the basis of data. We feel that meterologists and statisticians should be working together to clear up this confusion. It is very doubtful that either discipline could resolve this problem without the help of the other.

(i) page 105. Dr. Van Volkenberg asks the contractors to put their best advice into the (phase one) report and also to "comment on how successful it will be once you produce it".

Comments on the March 23/24 SCIREP Reviews

Again, because of the fact that we did not participate in the March 23/24 meeting, we found it necessary to read the SCIREP reviewers' comments in detail. Here we indicate only a few items that we wish to stress.

(a) Dr. Lamb expresses concern that the proposed approach is simply one of adding superficial features to two existing models that ERT already possesses. I share that concern. He also expresses the view that the value of the new models for decision making would be negligible.

(b) Dr. Mueller points out that the MOE objectives appear very ambitious.

(c) L.A. Barrie states that "more developmental research and less application of existing methodology is needed than is evident in this [first] prepared".

(d) Dr. Lumley states that while the first proposed "represents the current state of the art", it and other techniques in current use "suffer from common difficulties, most of which can probably not be resolved within the time frame of this project". He states "it will probably be possible to make some minor improvements".

(e) The present author has made two submissions prior to joining the SCIREP panel recently. These submissions, dated April (10 pages) and May (14 pages) deal with certain statistical problems and make a strong case that the contractors require the assistance of a statistician having suitable background.

Comments on the ERT/MEP Report Volumes

We have examined these three volumes (vol. I, vol. II, and Executive Summary Volume) but shall not be commenting on the purely meterological (chemical and physical) aspects. We shall mostly confine ourselves to the statistical matters that arise.

In Volume I we were favourably impressed by the proposed modularity of the system structure, by the segregation of the files and the general subsystem approach. Further opinion from a computing systems specialist could be desirable unless it were the case that the contractors have already demonstrated suitable capability in other similar computing systems projects.

Chapter 1 contains reference, to which I object, of "non-specialist users" who would be carrying out "routine modelling". There is nothing routine about modelling with an exceedingly complicated system and the myth that a non-specialist could do something useful with it should not be perpetuated. Any viable user would need to have a very clear grasp of the uncertainties inherent in the system and in its components.

We do not have any specific comments relative to chapters 2-9 for the reason given above.

Chapter 10 of Volume II gives the impression of coming from another report. This chapter considers in detail the effects of various simplifications to ERT's, SURADS nad PLMSTAR models, and in this sense, the title "model sensitivity analysis" is somewhat ambiguous. The simplified models are all compared to the complex ones, and this is our main criticism of this exercise. What is urgently required is a clear understanding of how these models (simple or complex) compare with reality. There is much discussion of SURADS and SHASTA and questions still remain about how much will be offered that is truly different and truly better. On page 10-185 some of the implications of the sensitivity analysis are brought together and are quite interesting.

Although the attempt to discuss concepts of model evaluation in Chapter II is an earnest one, we feel that serious limitations remain. We believe that ERT will need to obtain expert statistical help if they are to be able to cope effectively with this critical and major component of the project. We believe that the contractor is underestimating the importance and the difficulty of this phase.

To begin with whether the point is a very important one or not, someone is going to have to come out and say that the formulation of the framework on pages 11-1 to 11-5 is imprecise, garbled and confusing. And at the end it does not really accomplish a great deal.

The discussion following, concerning model evaluation, reviews protocal which is standard in the context of regression and normal distrubitions. The related discussion concerning the parameterization "p" is helpful. In particular, it is a neat point that "p" could be estimated using different sets of observations and that if the estimates displayed great variability it would call the model into question. A weakness of the discussion is that it is not clear just what "p" is in the context of this project. Further, a very serious weakness is that there is no attempt to discuss just what kind of data would be required, and how much computer and other time would be involved in an analysis of this for the proposed model.

A further weakness in the statistical discussion is the implicit reliance on "point" estimators without attention to their variability. It certainly makes the most sense that whatever is being estimated should be expressable in the form of a confidence interval. Failure to do so would, it seems to us, seriously undermine the credibility of the regulatory function.

The example which is discussed in section 11.4 is interesting but one should not be misled by the fact that the actual model here is very simple and that enough data were available to provide fully 66 independent tests of the model. The question of how to carry out an analogous procedure for the larger model being envisioned is not

addressed. Another important difference here is that the model examined in 11.4 is simply a regression.

The assertion on pages 11-20 that in practice "once a model is considered acceptable it is used on the assumption that model predictions deviate little from observations" leaves us feeling uncomfortable; this statement does not seem concordant with the regulatory setting.

Concluding Remark

We believe that the OME's objective No. 6 is at risk. Although the phase I report does discuss model evaluation in a general sort of way, no specific program is laid out for the determination of the uncertainties in the model outputs. There is also evidence in several parts of the report (eg. pages 1-50 bottom and pages 3-12 bottom) that the consultants are not dealing as effectively as possible with the elements of randomness. We think that it should be an absolute requirement that the contractors obtain suitable statistical assistance.

In view of the difficulty of obtaining suitable data, and the possible high costs involved in running the model, the quantification of uncertainty may be an undertaking which will require more planning than is evident in the Phase I report. The report does not discuss just what type of data will be required for this work, how many cases would be required, or just what might be involved in such an analysis.

8 October 1982

Our Ref: 120-10WP

Dr. R.D.S. Stevens
Organizer of the Peer Reviews of
the ERT/MEP Model System Design
Concord Scientific Corporation
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Downsview, Ontario
M3H 2V2

Dear Sam:

Re: Follow-up Comments to SCIREP Meeting of 23, 24 September

Thank you for the opportunity to participate in the last SCIREP meeting. My follow-up comments essentially echo those which I had set down prior to the meeting.

My principal concerns center mainly about MOE objective No. 6 which was regarded as being "highly desirable" by MOE: "The model is intended for regulatory application. Therefore it must accompany a clear statement of the uncertainties in the model outputs. The uncertainties must be quantified and protocol developed for regulatory applications of the model."

In their presentation, the contractors indicated that 35 - 40% of the model development task is taken up by model evaluation. However, chapter 11 of their report which deals with the evaluation questions constitutes only a very small percentage of that report. It is my opinion that if the objective No. 6 is to be taken seriously, then the project team should be augmented by the availability of a statistical consultant. This consultant should ideally have extensive experience and should have a justifiable, strong reputation - at least within the statistical community. I would like to stress that I do not doubt the capabilities of the consulting team to carry out much of the statistical work; indeed, there is evidence of considerable strength. The interactions that would develop with the suggested augmentation should however prove to be of great value, in my opinion.

Dr. R.D.S. Stevens
Concord Scientific Corporation

8 October 1982

During the SCIREP discussions, there was some brief consideration of the legal aspects of the regulatory process. I do not believe that enough attention was given, in this discussion, to the potentially adversary nature of this process. The questions of model uncertainty could play a very critical role here, and it is the statistical link which is likely to be the weakest one, and therefore the one which would be most open to attack. I do not believe that all the weakneses of this link can be resolved, but it would be creditable to those involved in the project if these difficulties could be documented in a frank manner, and discussed in relation to the state of the art in atmospheric modelling.

It is my hope that these suggestions can be favourably considered. I believe that the field of atmospheric modeling in its present state could benefit from greater interaction with the statistical discipline.

Sincerely,

Andrey Feuerverger

AF/lb

Comments On
Models for Long Range Transport . . .
ERT/MEP Reports, August, 1982
J. M. Hales

Executive Summary

In short the executive summary is a well-done and reasonable presentation. If it were to be read by itself, however, it would leave the reader wondering just how much of the material described here is to be developed under this program, and how much exists already. The next two volumes elaborate on this in detail, and so this isn't any real problem; but it should be kept in mind if the executive summary is to be circulated by itself. A second mild criticism is that the authors present a perhaps overly-optimistic picture of the utility of models on page 4.

Volume 1

1. OPERATING SYSTEM

This is an excellent idea and is well presented. The authors should be encouraged to bring this concept to an advanced stage of completion for use with not only the presently-envisioned models, but for other, more elegant models as they evolve. If completed as designed, this feature will save a lot of scientist-hours in future applications.

2. REVIEW OF WIND-FIELD MODELS

No comments required, owing to the fact that this is a review only.

3. WIND-FIELD MODELING FOR CURRENT PROJECT

This is well outside my field of expertise. As an outsider, however, this presentation strikes me as a well-designed approach, which makes about the optimal use of the state-of-the-art, without going overboard on esoteric concepts.

Volume 2

4. STRUCTURE OF LRT AND MESOSCALE MODELS

- The splitting of the LRT and mesoscale models into two categories is appropriate.
- The grid-point resolutions and spatial domains of the two models are appropriate.
- The computer resources estimates hinge somewhat on the idea of a "typical three-day simulation." I suggest that three days is too short for most LRT applications because the influence of the initial conditions (which are usually chosen arbitrarily) is still present under most circumstances at that time. Longer runs almost certainly will be necessary, and computer demands will have to be expanded accordingly.
- The vertical and horizontal coordinate transformations are appropriate.
- They have taken a logical approach toward handling the boundary conditions, including the outflow condition.

5. NUMERICAL METHODS

- This section begins by reporting the tests of essentially three different techniques for integrating the advection terms of the basic governing equation. The first of these is the SHASTA method, the second the MFCT Variation, and the Cubic Spline method is the third. Apparently the cubic spline method is the one to be applied for the OME model, but the text on pages 5-32 doesn't make this totally clear. They recommend, for example, that "further testing" be conducted. What kind of tests? What if the tests fail? This is an extremely important decision point, because it will be

difficult to reverse. Accordingly, it should be approached with utmost care. I'd also suggest that a contingency plan be formulated to cover the possible situation that some back tracking may be necessary.

- The diffusive terms are covered appropriately and, at any rate, are much easier to handle than the advection terms.
- The transformation terms are covered using an integration technique which is about optimal, given the present state of the art.

6,7,8. REACTION AND REMOVAL

These sections contain a substantial amount of review material which is utilized to formulate the attack for the present model. While all of this was pretty much on-target, I was struck by the imbalance between the complex approach to (especially homogeneous) kinetics on the one hand, and the relatively crude treatment of wet and dry deposition on the other. Certainly the approach to the removal phenomena is warranted by the low state of the art. But since this is true it may not be cost-effective to be overly detailed in the chemistry characterization -- especially when some well-designed lumping cloud have dramatic effects on computational resource requirements. I recommend strongly, therefore, that the authors seriously take the question of balance into consideration and attempt to optimally distribute the level of detail within their modeled system.

10 & 11. MODEL EVALUATION AND SENSITIVITY TESTS

Section 10 is a lengthy analysis of sensitivity of model output to changes in modeling assumptions and input drivers, using presently existing models. While this is a reasonable exercise to have performed it deserves little comment here, owing to its somewhat review-ish nature. A major finding of importance for OME work, however, is that major uncertainty exists in how

closely the numerical integration schemes are approximating the solutions to the governing equations -- this reflects back on my comments regarding choice of the integration technique, given above.

Final Comments on OME Modeling Program

J. M. Hales

My general impressions regarding the OME modeling program and contractor performance during its initial stages have been rather amply stated in my oral comments and in my review of the reports. In brief, I feel that the contractors have done a competent job and that the work should continue with the modifications indicated by the review committee.

It should be noted that if OME had the choice of drawing scientific talent from a diversified base of personnel, then the product would be potentially much stronger than will be the case under present circumstances. Thus it is easy for the committee (who itself represents a rather broad diversity of high-level talent) to criticize the work to date. It is my opinion, however, that the contractors provide about as good a base of skill as is possible when one is confined to the selection of only two groups. They should be allowed to proceed on a course which is rather carefully monitored, but which also has sufficient flexibility to enhance a creative approach.

The inclusion of consultants and subcontractors is a possible way to augment the program in a way which will boost some of its weaker areas. I recommend, however, that a cost-effective inclusion of such resource people will be a somewhat tricky undertaking, and should be treated with some caution. The reasons for this are as follows:

- In general the consultants that you will desire will be heavily committed to other projects, and thus time-allocation and conflict-of-interest problems will undoubtedly arise. It will be essential that the added personnel commit themselves to a significant block of effort, in order to make the program cost-effective. It is essential also that all conflicts-of-interest (eg., participation on competing modeling programs) be well resolved. This will be difficult because these other modeling programs are precisely where most of the desired personnel are expending their current efforts.

- Inclusion of this added talent for required time periods will be expensive. In order to make this inclusion more than sub-critical, however, these financial resources will have to be expended; otherwise the incremental funding will be almost totally wasted. I recommend, therefore, that OME consider the inclusion of sub-contractors very carefully, and not utilize this resource at all unless a critical effort can be realized.

40

U.S. DEPARTMENT OF COMMERCE
National Oceanic and Atmospheric Administrati
ENVIRONMENTAL RESEARCH LABORATORIES

Post Office Box E
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September 3, 1982 RD/RF326:BBH

32 REC'D

Mr. R. V. Portelli
Director Modeling and
Air Quality Assessment
Concord Scientific Corporation
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Downsview (Toronto),
Ontario, Canada M3H 2V2

Dear Mr. Portelli,

I have read the report accompanying your letter of August 12, and my review and recommendations are enclosed. On the whole, I am impressed by the game plan, and disturbed by the fact that the big model is made up of little models, which are sometimes made up of even littler models. At times, it seems hard to identify what we really know!

Sincerely yours,

Bruce B. Hicks
Director, Atmospheric
Turbulence and Diffusion
Laboratory

Enclosure

BBH:ss

P. S. Sorry it's so long, but I didn't have time to be brief!

SCIREP

Review and Recommendations

B. B. Hicks 3 September 1982

As far as I can tell the revised report is a superb explanation of the pieces that have to be put together to produce a comprehensive model of sub-continental scale transport, transformation and deposition of air pollutants. In this, I believe that this program has already been exceedingly profitable.

Having examined the various pieces that make up the submodels of this scheme, I am impressed with the overall concept. However I am struck by the similarity between what is proposed and "framework" models that have been put forward by the other workers, especially EPA/ESRL and MAP3S. These "framework models" are viewed by many as management tools, intended to point to deficiences in existing knowledge and to provide the conceptual link between the various research components. I subscribe to this view, for reasons that I hope to make clear.

Suppose we have a "perfect" model, with all of the submodels adequately representing their processes, interconnected correctly, and driven with suitable external information. The time and distance scales are such that we are dealing directly with the diurnal cycle, with all its variability and uncertainty. Even for daily averages, I do not believe that better than a 70% correlation coefficient between predictions and observations can be achieved, because we are at the mercy of phenomena that are randomly distributed in space and time and which cannot be simulated in an organized model. Hence, I do not have any hope that an episodic model can be developed.

This is not a great limitation, however. A complicated model can look at what controls the variance as well as mean values. It can relate sources to sinks, on the average but probably never for specific, short-term cases. The model is a necessary development, however, if only to augment statistical models and to test the importance of using more and more complicated submodels.

So, if the intent of this exercise is to develop a model capable of identifying particular sources with observations of severe pollution, then I regret that I cannot be overly optimistic. However, if the intent is to help identify deficiences in existing knowledge, to guide the development of better parameterizations of processes, or to attribute observations to source areas on the average, then I am quite confident. But it will be expensive!

By the way, I disagree with the introductory remark that a fully-developed parametric model of this kind is less susceptible to criticism. To my mind, any simple model can be criticized for the inadequacy of the modelers' attempts to simplify nature. In this case, the large model is no more than a sythesis of many simple models, and hence it

is much easier to criticize. The chain has many weak links. Let me point out a few, in the hope that they might be repaired a bit.

On many (if not all) occasions, the submodels are based on parameterizations that are appropriate in some circumstance, or are tuned to some specific data set and so far unverified.

1. The nocturnal PBL formulation leans heavily on the Coriolis parameter. This is good for some areas, perhaps, but I have been unsuccessful in every one of my attempts to verify it. Occam's razor says that f can be omitted.

2. The diurnal PBL scheme is not one that I have seen extensively tested.

3. The water-surface roughness formulation is open ocean. This is no big deal, but I think the text should consider inland waters separately if only to show that we know the difference.

4. The wet deposition scheme is an example of formulations that fit some limited data, on the average.

5. The dry deposition scheme seems not too bad, although I am worried that the models and data do not agree.

6. I cannot find a model component addressing clouds that do not rain.

7. All of this effort is at the mercy of the emissions inventory. How well do we know the SO_2 and SO_4 input rates? And how can MEP/ERT hope to improve on the MAP3S (SURE) EPA inventory?

8. The meteorological data is (as stated) gridded at about 500 km intervals. This means that we can only count on a few data points for each day of travel. This will serve to expand the diurnal variability, about which I was already insecure.

I fear that my major citicism is that the large model is made up of many submodels, each of which involves a new level of model, sometimes without any direct observations. We are building up a model out of other models. I always find this a little scary.

Recommendations.

This is the first time I have seen a comprehensive examination of all that might be involved in a model of this kind. The material convinces me that we cannot hope to do the job sufficiently well to talk about specific times or locations. However, it is not necessary to run a complicated model with all of its complexity at all times.

I feel that this model would make a powerful research tool, and recommend that work should continue. In particular, the model will permit us to examine the comparitive importance of different-processes in different circumstances. It might also be quite adequate for studying the consequencies of alternative control strategies.

I am sure that any of us could argue with almost any of the formulations used in the submodels, however I doubt that any of the differences that we might make would be critical. There are only a couple of places where the physics seems to be inappropriate, and it is in these cases that a change might be most desirable. In particular, I would modify considerably the PBL parameterizations that include Coriolis. Such relationships might apply in a continually neutral atmosphere, but surely not in the real mixed layer where controlling properties are the surface heat budget, radiation cooling, terrain complexity, and probably other factors that I have forgotten.

The dry deposition parameterization seems to emphasize physics rather than chemistry and biology. I appreciate that the fault does not lie with the present workers, but rather with other modellers who are addressing cases in which trees are rare and humidities are low, but we can certainly do better for eastern North America.

Likewise, the wet deposition parameterizations seem to emphasize particle scavenging by hydrometeor impaction and coagulation, rather than by humidity growth and nucleation followed by impaction, etc. Once again, I know that the fault does not lie with the present workers, but with the meteorological situations modeled by the workers whose results they are using. These results are probably quite appropriate for stratiform or orographic rain, but not (I suspect) for eastern North American convective rainfall. Snow presents a completely different set of problems that we also know a lot about.

I applaud the nocturnal "jet" emphasis, but regret that the results of the many North American field studies to investigate the problem have been bypassed in favor of using somebody's imaginative model. We have been conducting work on this subject for at least seven years now, and know that the georgraphical extent of the phenomenon is not limited entirely to the midwest. However, the probability of occurrence changes markedly as one crosses into the Eastern time zone. I recommend that the parameterization should include a spatially-varying probability distribution to simulate the observations so far. (This, by the way, is the subject of intense interest, but is presently unfunded by anybody. So we are all grasping at straws.)

Finally, because of the magnitude of the effort, I would be reluctant to duplicate ground-work completed elsewhere. For example, USDA have complete land use maps, and the Bailey ecosystem maps probably give good enough surface detail for anything related to biology. Since the

agriculturists and ecologists have already completed their mapping of the surface of North America, why attempt to do the job again? Moreover, I do not think that the satellite techniques can compete with visual observations and field reports.

Supplementary Comments on LRT Model Activity

In response to the request to consider whether the present modeling efforts will satisfy MOE requirements, the following points should be emphasized:

1. If it is the hope to develop a method to relate specific deposition occurrences to specific sources at regional-scale distances, then the chances of success are zero. It is impossible for an organized model to simulate the effects of a series of connected, random events (e.g. non-raining clouds, and precipitation patterns).

2. If the intent is to provide an improved method to assess the probability that an observed deposition event is related to some specific source, then the chances of success are high.

B. B. Hicks
20 September 1982

U.S. DEPARTMENT OF COMMERCE
National Oceanic and Atmospheric Administratio
ENVIRONMENTAL RESEARCH LABORATORIES

Post Office Box E
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September 30, 1982 RD/RF326BBH

OCT - 6 1982

Dr. R. D. S. Stevens
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Downsview, Ontario
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CANADA

Dear Sam:

Congratulations are due to you and your cohorts on an excellent meeting last week. A few reactions are given below, and some other past-meeting comments are attached. I have purposefully kept my material short.

1. I do not agree with a strong emphasis on statistics. For the individual parameterizations, uncertainties are provided by the experimentalists who developed the parameterization. For the final, simpler "progeny" of the fully expanded model, testing would be against network data, probably using one of the various techniques presently being discussed by the professional societies, EPA, etc. But to test the fully-developed framework model would require data that presently does not exist. So why fool ourselves? Why not support the continued association with the ongoing deliberations regarding model verification, with the intent of applying the best possible methods that are available in a couple of years time?

2. The role of a statistician at this time would be to ensure that uncertainties of the basic parameterizations are propagated through the model in an appropriate manner. I do not believe that we can afford to promote a model verification initiative that is independent of what the rest of the community is doing.

3. I would encourage the parallel development of a Lagrangian, statistical trajectory (or similar) model that could be used for simple application of the lessons learned by the framework exercise. Such a model is especially suitable for evaluating seasonal averages and statistical variability.

Dr. R. D. S. Stevens September 30, 1982

4. I am specifically against asking for an improved design document. The team has done an excellent job in responding to the first set of SCIREP recommendations. We have no reason to believe that this excellent precedent will not continue to be followed.

The narrative comments that are enclosed have been condensed from some more extensive notes I have. The larger wad of paper would be useful as a weapon, more than support for logical arguments. I will provide it if you wish to threaten people with the need to read inches of paperwork.

Sincerely,

Bruce B. Hicks
Director, Atmospheric
Turbulence and Diffusion
Laboratory

Enclosure

BBH:mr

Post-meeting comments — Bruce B. Hicks

1. A little history helps. The models used in the early US/Canada negotiations were essentially air-quality simulations, modified by the inclusion of a deposition routine selected at the whim of each modeller. The wide range of parameterizations used illustrated the uncertainty involved in formulating these processes. In the MOI work, there was no attempt to decide what constituted an acceptable parameterization. Instead, all of the outputs were given equal weight. This made it exceedingly difficult to defend the results obtained.

2. The Eulerian framework model is a critical development at this time. It provides the only way to compare the various parameterizations and the interactions between them. Without an Eulerian model, regulators and scientists alike will have no capability to evaluate the nationality of simpler models, and we will have no way to judge what chemical, physical and biological processes are overwhelmingly important, or sufficiently trivial that they might be omitted without loss of generality.

3. There are two basic questions that the regulatory models must address.
   a. What is the average situation over seasonal periods, and how is it changing?
   b. What is the probability that certain predetermined limits will be exceeded during shorter time intervals?

   Neither question requires the direct application of the Eulerian framework model, and I predict that it will never be used for these purposes. Instead, the results obtained using the Eulerian models will be applied as parameterizations in Lagrangian, simplified Eulerian, and/or statistical models, and used to interpret field data and extend them to other circumstances.

4. To address any of these questions, it is necessary to apply the fully-developed Eulerian models with care. We must ensure that model results are not dominated by a memory of the initial (or boundary) conditions. A three-day run does not seem adequate for this purpose. In practice, the model outputs should be able to reproduce the major features of the air pollution concentration spectrum, and so runs long in comparison to a synoptic cycle should be considered.

5. Several points should be made regarding the philosophy of testing the model. A typical experimentalist aims to produce an answer in the form of the most suitable formulation of the process they are investigating. If he follows the basic rules of good science, he presents his results in a way in which error margins are obvious. The Eulerian model contemplated here will combine sets of these formulations, to synthesize a more complex model of atmospheric behavior. This complicated model is made up of individual parts, each of which should be formulated by the "experts" who studied the process, with specified (or readily calculable) error margins.

Post meeting comments - B. B. Hicks

The major question of error margins that arises for the framework model concerns how these individual errors affect the quality of the overall model outputs.

Note, please, that I do no consider it a major goal of the framework modellers to develop new parameterizations from data. My experience has been that almost inevitably data is best analyzed and reduced by the "experts" who obtained the results. Otherwise, we are at the mercy of the imaginations of lesser experts. However, I consider it to be quite acceptable for a documented formulation to be modified in order to meet the structural constraints of some other model, provided this is done in a way that preserves knowledge of the uncertainties involved. From the viewpoint of the framework model, the testing of the individual modules should have already been done by the "experts" who developed them. (If not, then these "experts" ought to be taken to task. I fear that I might be one of them!)

However, this does not take care of the entire problem. We need to check the simplifications of initially complicated formulations, and we need to generate some faith in the quality of the outputs of the synthesized model. The first part is easy; the second isn't. To test the framework model would seem to require data from a dense network operated with hourly time resolution (perhaps) for "episodic" periods. To test the simpler models developed out of the framework model seems much easier -- seasonal averages and statistical variability seem important factors that can be evaluated from existing network data.

The framework model is an intermediate product that will be almost impossible to test thoroughly. However, we can test its sub-modules, and we can evaluate the performance of its simpler successors.

6. The descriptions of meso-scale meteorological modeling activities appeared somewhat deficient, and clearly require strengthening. It is not clear that the improvement will cause any great change in the statistical features of the predicted deposition. However, I am confident that average values will be affected.

U.S. DEPARTMENT OF COMMERCE
National Oceanic and Atmospheric Administratic
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Post Office Box E
Oak Ridge, Tennessee 37830

October 4, 1982 RD/RF326:BBH

OCT 14 1982 REC'D

Dr. R. D. S. Stevens
Concord Scientific Corporation
3 Tippet Road
Downsview, Toronto.
Ontario, Canada M3H 2V2

Dear Sam,

In case my viewpoints did not come through strongly enough at the Toronto meeting, let me emphasize that I am not in favor of making the LRT modeling effort include a dynamic meso-scale component. Such a model would be required if one wished to investigate mechanisms of precipitation scavenging or to explain why a given cloud delivered a specific concentration at a particular time. Any such program must be conducted hand in hand with observations, by workers at the forefront of their field. I would be much happier if the LRT model applied the results of such studies, rather than try to engage in them. These results can be incorporated statistically.

I believe that we need a "minimum acceptable parameterization" in all cases, and that the complexity of the individual models should be in balance. To divert effort into any research area would disturb the logical balance too much for my liking.

I guess this goes to show that I am a generalist, not a specialist until, of course, I start to specialize in making generalizations.

Sincerely,

Bruce B. Hicks
Director, Atmospheric
Turbulence and Diffusion
Laboratory

BBH:ss

UNIVERSITY OF WASHINGTON
SEATTLE, WASHINGTON 98195

Department of Atmospheric Sciences, AK-40

SEP 8 1982 RECD

September 2, 1982

Dr. R. D. S. Stevens
Concord Scientific Co.
2 Tippett Rd
Downsview, Toronto
Ontario
CANADA M3H2V2

Dear Dr. Stevens:

Enclosed is the copy of my review comments on the ERT Modeling Report (dated August 1982) for SCIREP. I have confined my review, at this stage, to the aqueous-phase chemistry aspects of the model.

I spent one day in reading the ERT documents and preparing my review statement, but I will delay billing you for this until after our September meeting.

Sincerely,

Peter V Hobbs

Peter V. Hobbs
Professor

PVH:rj
Enclosure

COMMENTS FROM PETER V. HOBBS, UNIVERSITY OF WASHINGTON, ON ERT DOCUMENT ENTITLED "MODELS FOR LONG RANGE AND MESOSCALE TRANSPORT AND DEPOSITION OF ATMOSPHERIC POLLUTANTS. PHASE 1: MODELING SYSTEM DESIGN (AUGUST 1982)

This short review is limited to Sec. 6.3 ("Aqueous-Phase Chemistry and Related Process

1. General Comment

The parameterization of the various processes in precipitation formation, and the link between these processes and acid rain formation in hydrometeors, are treated in a very elementary fashion in the ERT model. Since these topics are of critical importance to the overall objectives of the OME Program, it would be premature at this stage to pass judgment on the viability of the ERT proposal.

2. Specific Comments

Page 6-71. The selection of the rate coefficient of Maahs (1982) for the O_3 oxidation of S(IV) is unfortunate. This rate constant was no doubt selected because it is high--not because it is reliable. The reactant concentrations employed were far higher than atmospheric. Only the study of Larson et al. (1978) was conducted at atmospheric concentration levels. At the high O_3 levels used by Maahs, O_3 could be producing H_2O_2 in solution (i.e. the rate measured may not be the O_3 rate). Furthermore, Hegg and Hobbs (1982) found no significant evidence of a dominant O_3 oxidation mechanism from measurements in natural clouds, whereas, if the O_3 rate of Maahs were applicable it would have dominated. I agree that O_3 oxidation must be considered in any model. The point is that this rate constitutes a major uncertainty in the model at the present time.

Page 6-78. It is not clear whether or not S(IV) oxidation by N(III), specifically $NO_2(Aq)$, is being considered in the model. Given the second order rate constant of 3×10^5 (Schwartz and White, 1982 are cited), this reaction will have a characteristic time of ~13 hrs with regard to S(IV) oxidation and will thus be too slow to be of importance.

Pages 6-78 and 6-79. The neglect of the catalyzed O_2 oxidation of S(IV) is unwarranted. The reasons cited, that [Mn] and [Fe] are poorly characterized in the atmosphere and that the reaction is subject to inhibition, apply equally well to the soot catalyzed and O_3 reactions, which are apparently considered.

Page 6-79. The soot reaction will have a characteristic time for S(IV) oxidation of $\sim 10^3$ hrs, even under urban conditions. I cannot see that it has any significance in the atmosphere.

Pages 6-84 and 6-88. The review of previous modeling studies is incomplete in that it does not discuss the important recent work of Scott (Atmos. Environ. 16, No. 7, two papers).

Pages 6-87, 6-92, and 6-93. Insufficient information is given on the parameterization scheme for cloud chemistry. Apparently, clouds are modeled by bulk-phase chemistry and the presence or absence of cloud is arbitrary. [The section on wet scavenging (section 7) also does not really deal with parameterization of the precipitation process but rather with parameterization of washout ratios and scavenging coefficients]. The difficult task of parameterizing the precipitation processes, to permit estimation of deposition as a function of cloud physics parameters, has not yet been done by ERT. The coupling of such a parameterization with a cloud climatology, to allow estimates of transport and deposition over any trajectory on a synoptic scale, has also not been done.

9/1/82

P. V. Hobbs

OCT - 6 1982 RECD

UNIVERSITY OF WASHINGTON
SEATTLE, WASHINGTON 98195

Department of Atmospheric Sciences, AK-40

September 29, 1982

Dr. R. D. S. Stevens
Concord Scientific Co.
2 Tippett Rd.
Downsview, Toronto, Ontario
CANADA M3H 2V2

Dear Sam:

Enclosed is a brief summary of the principal comments I made on the ERT/MEP proposal at last week's meeting.

Also enclosed is a statement of my expenses.

Thank you for making the trip to Toronto so enjoyable. I look forward to working with you in the future.

Sincerely,

Peter V Hobbs

Peter V. Hobbs
Professor

PVH:rj
Enclosures

UNIVERSITY OF WASHINGTON
SEATTLE, WASHINGTON 98195

Department of Atmospheric Sciences, AK-40

COMMENTS FROM PETER V. HOBBS, UNIVERSITY OF WASHINGTON, ON ERT/MEP PROPOSED "MODELS FOR LONG RANGE AND MESOSCALE TRANSPORT AND DEPOSITION OF ATMOSPHERIC POLLUTANTS"

Summarized below are the principal comments that I made on the proposed modeling effort during the meeting in Toronto on 23-24 September 1982.

1) The ERT/MEP group is strong in the areas of homogeneous gas phase chemistry, numerical techniques, and in the handling of large models of the type required for this project. The team is less strong in heterogeneous and aqueous phase chemistry, mesoscale modeling and cloud physics. For part II of the proposed project I recommend that they add staff members trained in the areas of mesometeorology and cloud physics.

2) The uneven distribution of skills in expertise referred to above has resulted in an unbalanced representation of the major components of the model. Thus chemistry (homogeneous and heterogeneous) receives undue emphasis compared with the mesometeorological and cloud physics aspects of the problem. Whereas, the chemistry is nearly state-of-the-art and is included in close to full detail, the mesometeorology and cloud physics do not approach state-of-the-art. This violates the "first hike to the top of the mountain" philosophy that the Ministry has indicated it desires. Some suggestions for improvements in the mesometeorological and cloud physics sections follow.

3) The present mesoscale model stops short of predicting the locations of clouds and precipitation. Instead it is proposed to utilize observations to determine these locations and the intensity of the precipitation. This is probably not possible with the present observing network. In particular, no useful methodology

was given for locating the heights and depths of intermediate cloud layers; since this information is likely to be critical in determining the time and spatial scales for the conversion, transport and deposition of pollutants, it represents a major weakness in the proposed model.

I recommend incorporating into the long-range transport model a nested 3-D mesoscale model designed to predict the locations of clouds and precipitation. The mesoscale model should not be developed by ERT/MEP, rather they should adopt one of several existing models. However, they will need to add a trained mesometeorologist to their staff to ensure proper handling of the adopted model.

4) The cloud and precipitation physics aspects of the problem are treated very crudely in the present ERT/MEP model, and some important topics are completely ignored. At minimum, I would like to see a level of parameterization of the cloud physics equivalent to that used by Scott (J. App. Meteor., 17, 1978). The occurrence of ice crystals in clouds at suitable temperatures must be allowed for in the model (since this will have a dramatic effect on in-cloud conversion rates and scavenging). A cloud microphysicist should be added to the staff to be responsible for this component of the model.

5) It seems likely that if more detailed meso- and micro-processes are incorporated into the model, other portions of the model will have to be reduced in complexity. Consideration should be given to replacing some of the existing explicit chemistry by parameterization and/or empirical relations. For example, some empirical expressions for the rates of production of sulfates and nitrates in clouds and for the scavenging of these species are becoming available, and more should be forthcoming in the near future.

6) Given the changes to the model outlined above, I would expect that within 2-3 years the ERT/MEP team should be able to produce a transport model that is capable of giving a qualitative picture of acid deposition for both long and short range transport. Improvements of the model to the point that it can provide quantitative predictions will depend more on increased understanding of the chemical and physical mechanisms involved in acid deposition (which must come primarily through field studies) and on improved observational capabilities (e.g. the NEXRAD doppler radar network) than it will on numerical model development per se.

Peter V. Hobbs

Peter V. Hobbs
9/29/82

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
Research Triangle Park, North Carolina 27711

September 9, 1982

SEP 24 1982 RECD

Dr. Sam Stevens
Concord Scientific Corp.
2 Tippett Road
Downsview, Ontario
Canada M3H 2V2

Dear Sam:

My comments on the Phase 1 Modeling System Design report are enclosed.

If I had to appraise the meteorology section in one word, it would be "mediocre". Based on the impressions that I have formed from this document and the original one that we discussed in Chicago, I recommend that OME require that a meteorologist experienced in meteorological models be hired as a consultant to this project. I suggest Dr. Tom Warner, Dept. of Meteorology, Penn State University, University Park, PA 16802. He has considerable experience with mesoscale meteorological models and their applications to air pollution simulation.

I do not know what your future plans are for SCIREP, but if further work is planned, I would like to retire now from the committee. I find the review work very tedious and coming on top of the heavy modeling work load that I have here at the lab, it requires more energy that I seem to have available. I mentioned this to Ken Demerjian, since the Meteorology and Assessment Division is interested in this program, and he has indicated that someone else from the Division could participate on the committee if it were mutually desireable. I suggest that you contact him on this matter if there is any interest. I appreciate the opportunity that you gave me to provide input to this important program.

I will not be able to attend the upcoming meeting in Toronto, September 23 and 24. I hope you have a successful session.

Best regards,

Robert

Robert G. Lamb, NOAA
Meteorologist
Atmospheric Modeling Branch
Meteorology and Assessment Division
Environmental Sciences Research Laboratory

Enclosure

Comments of R. Lamb on "Models for long range and mesoscale transport and deposition of atmospheric pollutants: Phase I: Modeling System Design"

It appears that a great deal of effort has gone into the preparation of this report and for this its authors should be commended. I focused attention on the meteorology sections of the report and will comment on these below.

I did not understand why isentropic analyses were proposed for the meteorological fields. In precipitating systems air motions are not isentropic because heat is injected into the air by condensation, it is absorbed during evaporation, and there is radiative cooling at cloud edges. I also did not understand the proposed role of the isentropic analyses. As far as I was able to gather from the description, they play only a dummy role in the wind field construction.

The method proposed for computing vertical velocity is unsuitable for the intended application. Vertical velocities derived from the continuity equation under all the meteorological conditions that this modeling effort will address are generally unreliable, due primarily to errors in the divergence estimate. A much better method exists for estimating ω that also allows for the effects of diabatic heating to be taken into account. I leave it to the contractors to find this method.

Provision is made for making the horizontal winds consistent with vorticity and divergence estimates derived by supposedly independent methods, but no attempt is proposed to make the vertical wind and precipitation fields compatible. In fact, precipitation plays an incidental role throughout the meteorological analyses. In actuality the horizontal winds, the vertical wind and the precipitation fields are intimately connected. Unless some effort is made to ensure that the relationships among these fields satisfy physical principles, systematic errors can result in model predicted deposition patterns.

On page 3-42 it is stated: "Surface wind observations... are not generally representative of the regional surface flows"; and on the basis of this claim, surface wind data are completely ignored in the regional model. This implies that the mesoscale pertubations induced in the synoptic scale flow by terrain, changes in surface roughness and albedo, etc. have no effect on the fate of airborne pollutants. At the very least these mesoscale fluctuations in the horizontal flow would have a dispersive effect but no provision is described in the report for parameterizing them. The horizontal diffusivity is apparently treated either by a constant eddy diffusivity of $K_H = 10^4\ m^2\ sec^{-1}$, whose origin is unknown to me, or it is relegated to the status of truncation errors in the finite difference scheme and ignored altogether. Neither treatment is acceptable. Furthermore, the mesoscale fluctuations affect the rate at which the plumes from neighboring cities and sources mix and this has a significant effect on the average rates of nonlinear chemical reactions. But no provision is made to parameterize this. In the long range model, terrain plays no role at all because even in the proposed method of computing the vertical velocity, the vertical wind speed at the earth's surface is assumed to be zero everywhere. This procedure is at odds with current practice in meso and global scale meteorological modeling.

Brand Niemann sent me a paper this week in which he describes analyses of 4 years of MAP3S acid deposition data at 4 - 8 sites. He found that 30% of the total annual wet sulfur deposition at Whiteface Mountain in 1978 was contributed by only 3 of the 54 precipitation events observed that year. Moreover, these three events were of the isolated, convective storm type whose spatial scale was of the order of 10^4 km^2, i.e., one grid cell of the proposed long range model. Convective storm simulations are not mentioned in the proposal as far as I can tell, nor is the treatment of nonprecipitating clouds on sulfur chemistry. Questions that come to mind are: How are the bases and tops of convective clouds determined? How are the vertical fluxes of material from the mixed layer into the cloud layer parameterized? How is the liquid water distribution in the cloud layer estimated? How is the vertical air speed within cumulonimbus determined? In this connection it should be noted that often in regions where there is net upward motion over a large spatial region, the upward motion is concentrated within several cumulonimbus and outside these clouds there is subsidence. The subsidence acts to lower the mixed layer depth over a wide area around the convective storms, while strong low-level convergence sweeps material from the mixed layer and carries it through the storm to high altitudes. As a result of the low-level convergence, pollutants from an area much larger than the storm's base can be deposited within the relatively small area in which precipitation falls. In other words, ignoring the mesoscale circulation around the storm would tend to cause an underestimate of the acid deposition. None of the processes just described could be treated in the proposed model without suitable modifications.

ERT has done a good job of investigating finite difference schemes for use in the model. However, more testing should be done before final selection of the scheme. A necessary condition for a viable scheme is that its errors are not exacerbated by the chemistry. To check this, tests should be performed of the advection of clouds of the chemically reactive species that will be treated in the model. I should also point out that the tests reported in the document considered clouds no smaller than 2x2 grid cells. But with a cell size of 110x110 km as proposed in the long range model, plumes from major urban areas will be no more than a single cell wide. Truncation errors generated by concentration gradients this large will be severe and they will have a major effect on the chemistry. Cells this large will also give rise to significant subgrid scale chemistry effects associated with convective and orographic precipitation and especially with the emissions of large power plants. It may turn out that a smaller grid size is advantageous.

In summary, the meteorological portion of this proposal needs a lot more thought and work before I would consider it to be appropriate for use in a "state-of-the-art" acid deposition model.

September 8, 1982

Cornell University

Sibley School of
Mechanical and Aerospace Engineering
Upson and Grumman Halls
Ithaca, New York 14853

September 17, 1982

Dr. S. Stevens
Concord Scientific Corporation
2 Tippett Road
Downsview (Toronto)
Ontario, Canada M3H 2V2

Re.: Review comments on "Models for Long Range and Mesoscale Transport and Deposition of Atmospheric Pollutants".

Dear Dr. Stevens:

I feel that in this report ERT/MEP have made an effort to repond to the comments of the Scientific Review Panel. However, I still have grave reservations about one aspect of the modeling, and consequent serious doubts that the model as proposed will meet the objectives of the Ontario Ministry of the Environment.

My primary concern has to do with Section 6, Atmospheric Chemistry Associated with Acid Precipitation. In this section, the authors neglect the terms arising from concentration fluctuations. In justification of this, they say (p. 6-109) "Far downwind of the sources (100 to 300 km), concentration variations are generally small." I am not familiar with the data on which the authors base this statement. So far as I am aware, the question of whether the level of concentration fluctuations (relative to the mean concentration) goes to a constant or to zero far downstream of the source is a matter of current controversy, with the body of informed opinion on the side that the ratio goes to a constant. While not absolutely conclusive, if this is true (as seems likely) the effect of concentration fluctuations on the effective bulk reaction rate can never be neglected. Neglecting this effect, as the authors propose, would result in very serious errors in predicted levels. I do not feel that the proposed exercise (section 6.5) of the ERT PLMSTAR model with variable cross-wind resolution addresses this problem.

I have no real quarrel with the remainder of the proposed model. The proposed parameterization of wet deposition is probably the weakest area (after section 6), but I believe that it will be adequate.

Very truly yours,

John L. Lumley

John L. Lumley

Willis H. Carrier Professor
of Engineering

JLL/mm

Final comments on ERT/MEP Proposal

I am most concerned about the chemistry, which I am sure is excellent from a chemical point of view. My concern has to do with the effective bulk reaction rate, which would be given by (for a second order reaction).

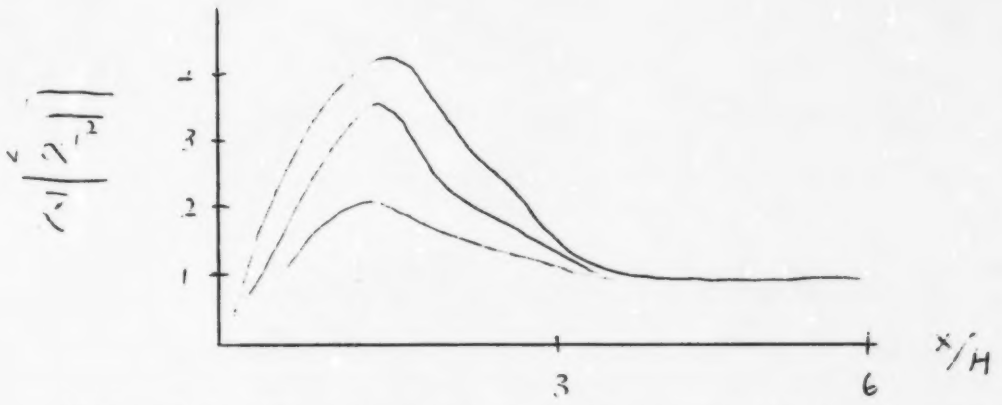
$$k\left(1 + \frac{\overline{\alpha^1 \beta^1}}{\bar{\alpha} \cdot \bar{\beta}}\right)$$

The authors admit that the term in $\overline{\alpha^1 \beta^1}$ could make a substantial change in the effective rate (the term can be written as

$$\rho \frac{\sqrt{\overline{\alpha^{1^2}}}}{\bar{\alpha}} \quad o \frac{\sqrt{\overline{\beta^{1^2}}}}{\bar{\beta}}$$

where ρ is the $\alpha \cdot \beta$ correlation coefficient; ρ is usually negative, and can be close to -1). However, the authors state that the fluctuations are negligible except near the source.

Everyting we know about the physics of plume dispersal indicates that this is not true. We are so acccustomed to dealing with Gaussian plume models that we tend to think that the instantaneous plume cross-section is Gaussian. This is not the case - the instantaneous plume is always relatively narrow, and meanders farther and farther from the centre line. This means that $\sqrt{\overline{\alpha^{1^2}}}$ and $\bar{\alpha}$ will always be of the same magnitude. Recent measurements bear this out. In particular, see Fackrell, J. and Robins, A. in both the Journal of Fluid Mechanics and Boundary Layer Meteorology 1982. They report measurements from an elevated source in a boundary layer made for the CEGB, which look something like this:



(The various curves corespond to various source sizes). By x/H = 6 the plume has filled the boundary layer vertically. There is no indication that $\sqrt{\overline{\alpha^{1^2}}} / \bar{\alpha}$ will ever decrease from unity.

There is also data of W.R. Moninger and Kropfli (Radar observations of a plume from an elevated continuous point source, NOAA/ERL) and other LIDAR data from NOAA/WPL of oil droplets that indicates the same thing.

Much of this is referred to in a document "Notes on B40 Convective diffusion experiment" by Julian Hunt, issued by WRL/NOAA, which has been given to Venkatram.

I feel that if no attempt is made to parameterize the effect of the term in $\alpha^1\beta^1$, the predicted levels will be very seriously in error. On the other hand, it seems to me that the parameterization should not be too difficult in the hands of a good theoretician. I cannot think of anyone better qualified for this work than Julian Hunt, who is already an ERT consultant; I suggest that ERT make better use of him in this connection.

J. Lumley

9/29/82

EPRI

SEP 24 1982 REC'D

17 September 1982

Dr. S. Stevens
Concord Scientific Corp.
2 Tippet Road
Downsview, Ontario
Canada

Dear Sam:

This letter constitutes a brief initial review of the ERT and MEP reports on Modeling System Design.

As per prior agreement with you, also please be informed that during a visit to EPRI on 9/15/82, Dr. Lavery of ERT presented a seminar on the work. During the question period, comments from EPRI staff were made on particulate matter deposition theory near the ground, on the production of H_2O_2 in cloud droplets, on the "Staubsauger" concepts of Crutzen's, and on differentiating processes that incorporate sulfates, nitrates and ammonium into rain from those that incorporate iron, calcium, magnesium, etc. We also mentioned the need to incorporate soot somehow.

I have scanned all those documents but am concentrating my attention on Chapter 6. Overall, very substantial progress has been made conceptually since our last meeting. While the design of the modeling system is really not complete, OME has probably obtained as much as it could expect. I anticipate that OME will be advised to follow up on the design work by going into an interim phase that would improve on the conceptual design and develop some of the specific submodules mentioned with respect to Task EI, Task MIV and Task MV.

I hope to have more detailed comments at the time of our meeting in Toronto. See you then.

Sincerely,

Peter

Peter K. Mueller, Ph.D.
Environmental Physics and Chemistry

PKM:ms

To: Sam Stevens, Concord Scientific
From: Peter K. Mueller
Subject: Comments on Model Design

I would prefer to send you my written comments by the end of next week rather than a hurriedly hand written draft prepared here.

To meet your immediate needs I am herewith providing my conclusions concerning the adequacy of the Model Design in relation to the OME objectives. As a result of the SCIREP meeting, I confirm the conclusion I came to in my letter of 9/17/82 to you.

A number of modules and sub-modules have been identified as being uncertain and untested. As part of the design work these need to be tested and decisions need to be made as to which formulation to include in the model.

I would like to encourage OME and associated sponsors to ask the principal investigators to continue the design work for the next year and to come back with a document that clearly identifies each module and sub-module to be used and the rationale for its selections. It should also demonstrate that the implementing computer codes work, in fact, as intended.

When this next step in the model development has been completed, the reports can be sent to the members of SCIREP for review and written comment.

In fact, as work on specific modules and sub-modules is completed it could be reviewed by the respective specialists on SCIREP. This would provide a means of continual feedback to the principal investigators, and serve as a stimulus to their work. Another meeting of SCIREP may then not be productive until 1 or 2 years from now. By that time each of the SCIREP members will have been involved with major advances in this field, which may then be worth discussing in a group setting.

To: Sam Stevens, Concord Scientific
From: P.K. Mueller
Subject: OME Project Discussion with Contractor

On 9/23/92, mid-afternoon, when the meeting with contractors was adjourned, I discussed with George Hidy the objectives and Tom Lavery's contentions that they could be met. I passed on to him my notes of Greg Van Volkenberg's four levels of achievement which were enunciated by him at the outset of our meeting on 9/23/82. He and I then discussed the status of the modeling design work in terms of Level 1 achievement and I requested that he discuss with Lavery, the ERT attitude to tell OME (or any client) what it wants to hear. I felt strongly, knowing what ERT can really do and Lavery, that he was promising authoritatively more than will really be delivered.

If OME accepts that, then just more noise than light will be added to the already very noisy world on the issue of acid precipitation. I advised him that ERT had done a good job as far as it goes, but much more design work was needed and ERT should advise OME forthrightly. He seemed to be acceptive to this advice.

National Agency of Environmental Protection
AIR POLLUTION LABORATORY
Risø National Laboratory
DK-4000 Roskilde, Denmark
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SEP 15 1982 RECD

Date 2 September 1982

Ref. No. 1396 mb

Concorde Scientific Corporation
2 Tippett Road
Downsview, Toronto
Ontario M3H 2V2
CANADA

Review of the Phase I Modelling System Design report prepared by ERT and OME for the Ontario Ministry of Environment.

The report entitled "Models for Long Range and Mesoscale Transport and Deposition of Atmospheric Pollutants" consists of three separate documents. Within the short time-limit for review of the documents, I have only been able to read through the documents very quickly. I will, therefore, give here the summary of my judgements, while detailed technical comments and suggestions for modifications will be discussed later.

The comprehensive reports give a detailed and excellent proposal for most aspects of the model development. It should be expected that the models developed on the basis of the suggested procedures, with some modifications, will give a new and improved tool for analysis and forecasting of acid deposition.

It is therefore recommended that the project be initiated.

Further discussions will be undertaken during the review meeting the 23rd and 24th of September.

Sincerely yours,

Lars P. Prahm, D.Sc.
Head of Meteorology Section

SEP 27 1982 :CD

Copenhagen, Denmark
September 1982

COMMENTS ON MODEL SYSTEM DESIGN OF MODELS FOR LONG RANGE AND MESOSCALE TRANSPORT AND DEPOSITION OF ATMOSPHERIC POLLUTANTS (AUGUST 1982)

by Lars P. Prahm

The comments are hereby given in relation to the 8 objectives laid down by the Ministry of Environment, Ontario.

Objective 1 & 2

Objective 1 and 2 state that the model to be developed should be able to give air concentrations of sulphur oxides and oxidants as well as deposition on a 24-hour basis through episodes and through whole years.

Experience with the SURAD model shows that the fully implemented model would require 20-100 CPU hours for a 24-hour run. It is expected that improvement of the numerical algorithms and implementation can reduce this with a factor of 3. This means that the model can not be used operationally on a scalar computer. A vector processor might speed the model up, but with no more than a factor of 10.

Based on these considerations, it is concluded that significant effort must be put into simplifications of the formulations of the physics and chemistry, and into development of advanced numerical algorithms. It is, however, the opinion of the reviewer that simplifications of these physical and chemical formulations could be made without reducing the capability of the model to treat the problem adequately.

Improved numerical methods are presently being developed, e.g. variable formula, variable step-size time integration of partial differential equations. Such methods might be introduced.

Objective 3

A mesoscale model of similar type, but with a grid point distance of about 10 km., will require about 10 times more CPU time for the transport part of the model. Even with a vector processor, such a model might use too much CPU time for operational runs. Significant simplification of the representation of the physics and chemistry and improvements of the numerical algorithms will be required.

Objective 4

The boundary layer parametrisation described in different chapters is not consistent. This problem, however, could be solved.

The reviewer is somewhat sceptical about whether the best available scientific knowledge is used in the field of numerical algorithms. But if problems should arise on this point, they could be solved. Other aspects should be considered by other reviewers.

Objective 5

It is expected that the contractor can implement the model for operational use. However, the sparsity of the meteorological parameters measured and the density of meteorological stations causes significant problems. It might be preferable to use output from the routine numerical weather forecasting models for the long range transport model. It is not clear how meteorological data for the mesoscale model should be obtained with a space resolution of about 10 km.

Objective 6

It is expected that even with the simplifications which might be introduced in accordance with the above comments, the contractor should be able to produce

a model which can be used for regulatory purposes.

Techniques for quantification of uncertainties are given in the proposal.

It might be useful to test the models on European EMEP data if sufficient data can not be obtained in North America.

Objective 7

The formulation of the model development gives good possibilities for test of different modelling procedures.

The reviewer is strongly biased in favor of the accurate and computationally fast pseudospectral numerical algorithms which have been developed and implemented during the last few years. It is suggested that these algorithms could be used as an option.

Objective 8

Detailed treatment of receptor areas of special interest should be possible if meteorological observations are available.

Conclusion

The model system design deals with a large number of different elements which have to be incorporated in the models. Although great difficulties exist with

respect to computational effort, it is expected that an LRT model satisfying the given objectives can be developed.

The development of a mesoscale model should be considered primarily as a research topic. Long term runs which include all elements of the described model might not be possible.

It is expected that the project will lead to useful tools for regulatory purposes, and it is recommended that the project be initiated.

Addendum

Based on ongoing work at the Danish Air Pollution Laboratory, the reviewer has some optimism with respect to the possibilities of obtaining fast and accurate numerical methods for the air pollution models. One should be aware, however, that it requires great effort and highly specialized experts to develop efficient numerical codes.

Comparisons of computational efficiency should be based on simultaneous consideration of:

a) accuracy

b) speed

c) number of grid points.

The conventional rotation test originally used by Crowley (1968) and Molenkamp (1968) has been used by several researchers. The report by ERT refers to tests by Chuck and Dunker (1982). We have repeated their tests and find that our pseudospectral code uses about 20 CPU sec (IBM 3033) for one rotation, while the fastest method by Chuck and Dunker (1982) is SHASTA, which uses 22 CPU sec.

Our pseudospectral code is thus not only more accurate, but also faster than the SHASTA code if the same number of grid points are considered. The pseudospectral code, however, shows good accuracy even with twice as large grid point distance, which would result in about 8 times less computational time for our pseudospectral code.

3-D tests with the SURAD model require about 360 CPU sec (IBM 3033) for a 24-hour run. This model works with 2 components and 23 x 30 x 5 = 3450 grid points. The 3-D pseudospectral code with 2 components

and 32 x 32 x 9 = 9216 grid points uses about 100 CPU sec pr. 24-hour run (average for February 1979).

This computational time is decreased with a factor of about 2 when variable formula variable step-size time integration is used. This amounts to 19 times less CPU time pr. grid point.

If the high accuracy of the pseudospectral code is considered and the horizontal grid point distance is doubled, we get a further reduction of CPU time with a factor of about 8.

In summation, existing codes can be used with a saving of computation effort on the transport part which accounts for a factor of about 150.*

* This estimate is based on the assumption that grid point distance and wind speeds in the SURAD and PS model were equivalent. Another factor of [illegible] can be obtained as a consequence

Lars P. Prahm

Copenhagen, Denmark

Comments added after SCIREP meeting

Toronto, 22 to 24 September, 1982

I LRT MODEL

It is recommended to initiate the LRT model development, if certain improvements are made. The LRT model is expected to be a valuable tool for qualitatively and perhaps some preliminary quantitative evaluation of long range transport of pollutants. The LRT model is thus expected to become a useful tool for environmental control. The LRT model is expected to be a significant improvement compared with existing models.

Recommendation

It is recommended that the LRT model is developed. This recommendation, however, is based on the requirement that certain necessary modifications are made:

1. Only short term (2-4 days) model runs are not adequate. Seasonal and yearly time integrations must be made. Long term averages should not be made on the basis of a limited number of episode studies.

2. Model results must be independent of initial conditions, which means that a model run requires a start up period of about a week.

3. Model evaluation should be made by comparison of model results which are independent of initialisation.

4. Re-initialisation should not be made. The limited life-time of the different species and correct implementation of numerical algorithms ensures stability of the time-integration.

5. Windfields should be constructed using standard procedures from the routine weather services (see comments by Anton Eliassen).

6. Windfields for the LRT model should be produced for several levels e.g. analysed 10m winds, 900 mb, 850 mb and 700 mb, and perhaps 500 mb, winds.

7. There is no need for further statistical expertise in the project team.

8. Treatment of the turbulent reacting regimes is a research topic of great interest, but it is not likely to be possible to be incorporated in the present project. If Professor Lumley can work out practical procedures to account for these aspects of the physics it would be useful.

9. The LRT model should be tested on the largest existing database from the EMEP project (European Monitoring and Evaluation Project). This database contains SO_2 and SO_4 24 hour air concentrations as well as sulfate in precipitation at about 40 stations through several years.

10. If data from other projects are used, quality control should be made, including inter-laboratory tests.

11. It might be useful to develop a highly sophisticated model, which requires meteorological input of higher space and time resolution than can be obtained for routine operational runs. Such a model might also use more computertime than

possible, if long term runs were produced. However, such a model must be considered as a research too. Such a model cannot be evaluated on a long terms basis, but it can be used to compare with models which are somewhat simplified. It cannot be used for long term integrations and thus cannot give the informations which are required for environmental evaluations and control.

II MESOSCALE MODEL

A mesoscale model can be made in two different ways:

1. One type is based on meteorological informations with detailed space resolution down to 10-30 km in the horizontal and about 100 m in the vertical, within the boundary layer. Such a model contains non-adiabatic treatment of the vertical motions.

It is expected that this type of mesoscale model can only be made on the basis of a dynamic meteorological mesoscale model because we have no meteorological observations of the required type and space as well as time resolution.

The reviewer finds that it is not possible to develop a dynamic mesoscale model within this project. Existing models at NCAR or British Meteorological Office might be used for certain limited regions for certain selected days.

However, long term air concentrations and depositions cannot be computed in this way.

The reviewer finds that Environmental Agencies should consider such studies as research and not as an operational tool. Furthermore, it is doubtful whether this detailed space and time resolution is of primary environmental importance presently.

2. In some areas, however, information of air concentrations and depositions are wanted with a space resolution of 10-50 km.

This type of information can be produced from a less sophisticated mesoscale model. It requires emission informations, precipitation fields and land use informations with the given resolution. The mesoscale model could then be made essentially by scaling down the LRT model. The wind field could be produced to some extent by interpolations from the field jroduced in the coarse grind system.

This type of mesoscale model can be developed and might give useful information for environmental evaluation and control.

Recommendations

It is recommended that this type of kinematic mesoscale model is developed.

Proper resting of the LRT model grid and the mesoscale grid should be made.

To ensure that state of the art methods are used throughout the project, it is recommended that a follow up review committee is created. This group should follow the model development and continuously support with advices.

CALIFORNIA INSTITUTE OF TECHNOLOGY

PASADENA, CALIFORNIA 91125

CHEMICAL ENGINEERING 206-41

August 23, 1982

AUG 30 1982 REC'D

Dr. R. D. S. Stevens
Concord Scientific Corporation
2 Tippett Road
Downsview (Toronto) Ontario
CANADA M3H 2V2

Dear Sam:

Enclosed are my comments on the ERT/MEP work plan. As you will note, I am impressed with the depth and detail of the plan and recommend strongly that the project continue.

See you on September 23.

Best regards,

John H. Seinfeld
Louis E. Nohl Professor
and Executive Officer

JHS:lk

Enclosure

Comments on

Models for Long Range and Mesoscale Transport and Deposition of Atmospheric Pollutants. Phase I: Modeling System Design, August 1982

J. H. Seinfeld

General Comments

The proposed plan is well conceived and thoroughly documented. Each section is based on a review of state-of-the-art understanding and contains well-documented conclusions. I found no major weakneses in it, and strongly recommend its execution.

Specific Comments

Page

1-50 The discussion of exactly how the emission inventory information is to be used is inadequate. The investigators will have to face this issue during the course of the work. The key questions that were not answered in the work plan were:

1) How will the total hydrocarbon (HC) emissions be allocated among species for the kinetic mechanism?

2) How will ambient HC levels be allocated among species for boundary and initial conditions?

3) How will primary sulfate and other particulate emissions be used in the model?

1-53 Characterizing the uncertainties associated with the emission inventory will be an important component of the sensitivity analysis and the evaluation of model performance. Greg McRae and I have recently worked out a way to estimate such uncertainties. A copy of the paper is enclosed for the ERT/MEP team.

1-55 Are the MAP3S data of value here?

1-75 It is not clear exactly how precipitation events will be handled. When simulating a past event, precipitation records can be used so that the treatment is deterministic. Is a stochastic treatment also envisioned?

5-1,2 These two pages are missing in my copy.

6-38 In Reaction 28, what is the basis of the choice of $k_{28} = 3.1 \times 10^{-6} T^{-1}$?

6-39 Same question for k_{37}.

6-39 I would like to have an explicit derivation of the stoichiometric coefficients in the lumped $\geq C_4$ alkane portion of reaction 33 (I need this for some other research I am doing on that mechanism anyway.)

6-48 How will emissions estimates be obtained for biogenic HC's?

6-92 How will the model utilize cloud droplet size distribution? Where will this distribution come from?

6-109 The Fisher (1981) reference is not included in the list of references. The problem of accounting for the effect of turbulence on chemical reaction rates is one of the most difficult in the entire scope of LRT and mesoscale modeling. Often it is difficult even to estimate whether the effect is important or not, much less developing a theory to include the phenomenon in models. I agree with the approach suggested on page 6-111 that essentially defers consideration of subgrid scale effects until Phase II. The use of PLMSTAR at that point, however, may not necessarily be the best approach. (See comments below.) In any event, subgrid scale chemical effects need not be considered in Phase I.

10-97 Section 10.2.1.1 The PLMSTAR reactive plume model has a number of technical deficiencies that may require redevelopment of the reactive plume model. Since that aspect is not proposed to be considered until Phase II, it is not necessary to include study of the reactive plume model in the current document. In short, reactive plume models such as PLMSTAR, and there are several in the literature, oversimplify the actual physics occurring and can be improved. As the project proceeds, I will be happy to discuss the reactive plume problem with ERT/MEP when it becomes of importance.

CALIFORNIA INSTITUTE OF TECHNOLOGY

PASADENA, CALIFORNIA 91125

CHEMICAL ENGINEERING 206-41

OCT -4 1982 RECD

September 28, 1982

Dr. R. D. S. Stevens
Concord Scientific Corp.
2 Tippett Road
Downsview(Toronto), Ontario
Canada M3H 2V2

Dear Sam:

Enclosed please find:

1. Report from SCIREP meeting
2. Statement of expenses

Sincerely,

John H. Seinfeld
Louis E. Nohl Professor
and Executive Officer

REPORT FOR SCIREP MEETING

September 23-24, 1982

John H. Seinfeld

This report will focus on evaluating the possibility of meeting the MOE's objectives. The comments below correspond to the revised objectives handed out during the meeting.

1. It should be understood that the model to be developed is primarily an episodic one ideally suited to simulate events of two to three days to one week duration. Although I expressed pessimism at the meeting concerning the possibility of exercising a model over a time period of one year, I was encouraged to hear of the European experience with models containing complex chemistry but simpler meteorology. Thus, I feel that this model can eventually be used to produce yearly average deposition values, however, it will not be a straightforward matter to exercise a model of this complexity for a time period of a year. Nevertheless, it is a worthwhile objective and an important one from the regulatory point of view. It is, in fact, one aspect of this project that may rightly be termed frontier research, that is, the exercise of such a model over a one-year time period.

2. In extensive discussions I had with Greg and P.K. after the meeting, I tried to convey what I understand to be meant by the term mesoscale as used in the objectives. In short, I understand mesoscale to refer to processes occurring on a spatial scale the order of one or several grid cells. From our point of view, the key processes occurring on these scales are cloud formation, vertical flows and precipitation. Since the primary object of this model is to simulate deposition, an accurate and careful representation of the mesoscale deposition processes is, as we all agreed, key. The project team needs to demonstrate whether a detailed mesoscale dynamic model

(e.g. Anthes) is needed or whether a data-derived empirical approach to generating cloud coverages, thicknesses and precipitation intensities will suffice. Thus, I recommend that the team first carry out a preliminary deposition model development, a time period required for which I would estimate to be about six months, then to determine whether more sophisticated mesoscale modeling is needed based on how sensitive the deposition calculations are to knowing the details of the cloud formation and precipitation processes.

3. The only area in which the best available scientific information was not apparent was that of cloud formation and the deposition process. I recommend that a consultant with the appropriate expertise be engaged by the team to assist in this area.

4. I am confident that the model can be programmed in a computationally optimal manner. This point should be conveyed to the project team.

5. The model must be used eventually for regulatory application. It would seem that the major aspect of the model for such application is development of the capability to simulate yearly average deposition values. It is understood that as a result of sensitivity analysis the model will be accompanied by a statement of the uncertainty in the predictions. At some later stage, it will be useful to have a consultant statistician spend a few days to look at the statistical aspects of the work. I am, however, basically comfortable with what Venkatram has proposed in this area.

6. The model is ideally suited to determine the impact of source areas on receptors.